

1-Propanol, 2,2'-oxybis-

Other names:	2,2'-oxydipropanol
Inchi:	InChI=1S/C6H14O3/c1-5(3-7)9-6(2)4-8/h5-8H,3-4H2,1-2H3
InchiKey:	VMKMZRBPOSNUMX-UHFFFAOYSA-N
Formula:	C6H14O3
SMILES:	CC(CO)OC(C)CO
Mol. weight [g/mol]:	134.17
CAS:	108-61-2

Physical Properties

Property code	Value	Unit	Source
gf	-383.88	kJ/mol	Joback Method
hf	-614.41	kJ/mol	Joback Method
hfus	13.61	kJ/mol	Joback Method
hvap	63.94	kJ/mol	Joback Method
log10ws	-0.17		Crippen Method
logp	-0.235		Crippen Method
mcvol	113.010	ml/mol	McGowan Method
pc	3853.09	kPa	Joback Method
rinpol	1041.90		NIST Webbook
rinpol	1075.00		NIST Webbook
rinpol	1036.00		NIST Webbook
rinpol	1075.00		NIST Webbook
rinpol	1036.00		NIST Webbook
rinpol	1041.90		NIST Webbook
ripol	1892.00		NIST Webbook
ripol	1892.00		NIST Webbook
tb	542.58	K	Joback Method
tc	705.59	K	Joback Method
tf	271.25	K	Joback Method
vc	0.415	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	278.16	J/molxK	542.58	Joback Method
cpg	286.98	J/molxK	569.75	Joback Method
cpg	295.49	J/molxK	596.92	Joback Method
cpg	303.67	J/molxK	624.08	Joback Method
cpg	311.54	J/molxK	651.25	Joback Method
cpg	319.10	J/molxK	678.42	Joback Method
cpg	326.35	J/molxK	705.59	Joback Method
dvisc	0.1960058	Paxs	271.25	Joback Method
dvisc	0.0181938	Paxs	316.47	Joback Method
dvisc	0.0030600	Paxs	361.69	Joback Method
dvisc	0.0007649	Paxs	406.91	Joback Method
dvisc	0.0002523	Paxs	452.14	Joback Method
dvisc	0.0001018	Paxs	497.36	Joback Method
dvisc	0.0000478	Paxs	542.58	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C108612&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature

tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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